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NEWS

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NEWS

This column regularly reports significant developments in the program of the National Standard Reference Data System. The NSRDS was established in 1963 by the President's Office of Science and Technology to make critically evaluated data in the physical sciences available to science and technology on a national basis. The System is administered and coordinated by the National Bureau of Standards through the NBS Office of Standard Reference Data, located in the Administration Building at the NBS Gaithersburg Laboratories.

NSRDS Status Report

NBS Technical Note 448, *Status Report—National Standard Reference Data System, April 1968*¹ (70 cents), summarizes the status of activities of the Office of Standard Reference Data. The report provides a detailed review of data compilation activities within the program's seven broad categories: nuclear data, atomic and molecular data, solid state data, thermodynamic and transport data, chemical kinetics, colloid and surface properties, and mechanical properties. Progress in data systems design and development and in information services of NSRDS are also reviewed. Certain problem areas of the program are identified in the report. The appendix lists information and data centers associated with the Office of Standard Reference Data, NSRDS publications, and organizations, groups, or individuals compiling or evaluating data.

This publication reports the progress made by the Office of Standard Reference Data in developing NSRDS. Since the program came into existence in 1963, the magnitude of the effort required to implement the System has been estimated more closely, procedures for the establishment of data centers have been developed, and relationships with other agencies have been more clearly defined. The Office has learned that the task of carrying out a critical evaluation is more demanding of both time and intellect than most members of the technical community undertaking these jobs had thought. The tasks involved have been clarified, and the qualifications of the staff needed within the data centers have been better formulated.

The original emphasis of NSRDS was on the production

of compilations of critically evaluated data, with a somewhat lesser emphasis on the production of critical reviews. Operating experience has shown that emphasis must also be placed on critical analysis of the sources of uncertainty in the measurement results reported in the literature. Estimates made of the fraction of the literature in any specific field containing data worthy of a detailed critical evaluation range from approximately 50 percent down to a low of only 8 or 10 percent. The Report indicates that in almost every field in which a reasonably common measurement technique is employed, criteria need to be developed for the conditions under which experimental measurements should be made. Additional criteria should be developed for reporting experimental results in the literature. Procedures are needed to ensure that results of quantitative measurements are made available to the data analysis center, even though they may not be reported in formal archival literature. In each of the fields in which the Office is active, the Report states that these needs will be examined in detail.

NSRDS progress has been slower than desirable; initial plans called for much more rapid development. The rate of development has, of course, been determined by the System's financial resources, which have been only a relatively small fraction of the estimated amount needed to accomplish the desired task expeditiously. Nevertheless, many useful products have appeared. When this Status Report was written, 31 separate compilations and 6 critical reviews had been published or were in press; 16 non-critical compilations or bibliographies have appeared. Others are in various stages of preparation.

As these products appear, the Report states, greater attention is being paid to the general problem of making them as readily accessible to the technical community as possible. In business terms, this is a marketing problem. The Office of Standard Reference Data has asked the question, "How should we market our products and services in order to accomplish the most good for the progress of science and technology in the United States?" The Office believes that a variety of marketing procedures must be employed, and it is gathering the information needed to develop plans for operation.

PRECISE: A Multiple Precision Version of Omnitab

One of the more troublesome problems that confront the careful user of modern computers is the loss of significance resulting from round off and other computing pitfalls. In many calculations rounding errors are serious sources of annoyance—in some they throw the results completely off. While the recent trend to design computers with built-in hardware for double-precision operations is a decided help in this regard, the user of these features must still be on guard. He must guard against possible flaws in the hardware or algorithms, and even, unhappily, against errors in important constants used by the compiler or the conversion routines.

The problem has become more serious recently because many of the third generation computers have a shorter word length. As a result, programs which previously gave suitable answers in single precision now must be run in double precision.

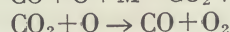
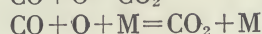
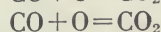
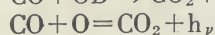
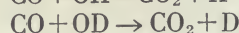
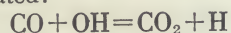
Soon after the proving out of the Omnitab² general-purpose computing program, effort at NBS was turned to the design of a comparable system for more precise calculations than were then possible in single precision. This system drew heavily on the multiple precision package previously designed by Alfred E. Beam of the University of Maryland. This package spares professional programmers the tedium of writing painstaking instructions for the computer to handle double and triple precision and out-of-range arithmetic. NBS Technical Note 446, *PRECISE: A Multiple Precision Version of Omnitab*¹ (55 cents), by Alfred E. Beam and Joseph Hilsenrath, describes how the package has been used to provide nonprogrammers with a computer tool for very precise calculations without resorting to conventional, tedious programming.

The PRECISE program was designed to carry out arithmetic operations and function generation, often to as many as 28 significant digits and at the very least to 21 figures. Except when instructed to increase the ranges, the program normally handles any number in the range $10 \exp(-76)$ to $10 \exp(76)$ and gives results to 28 significant figures. The program can also handle numbers outside of the above range. The greatest or smallest power of 10 can be as high as plus or minus one billion. In this extreme case the results are good only to 21 significant figures.

High Temperature Rate Data

The Department of Physical Chemistry, The University, Leeds, England, has just issued the report, "Critical Evaluation of Rate Data for Homogeneous, Gas-Phase Reactions of Interest in High-Temperature Systems," by D. L. Baulch, D. D. Drysdale, and A. C. Lloyd. In this report the rate data are tabulated, paper by paper, together with an indication of the method used and the evaluators' comments. These data and the recommended rate coefficient are also graphed.

The available rate coefficient data for the following reactions are evaluated:



A discussion and a bibliography are provided for each reaction.

This work is part of the High Temperature Rate Data Project supported by the U.K. Office of Scientific and Technical Information, which administers the British Data and Information Program. This Office is the U.K. equivalent to the NBS Office of Standard Reference Data, which administers the U.S. NSRDS program. Further information about the work of the Leeds Group or copies of reports may be obtained from Dr. D. L. Baulch, School of Chemistry, The University, Leeds, 2, United Kingdom.

Nuclear Magnetism to be Reviewed

L. H. Bennett, Director, Alloy Data Center and Chief, NBS Alloy Physics Section, has been selected to write Chapter 14 on "Nuclear Magnetism" in the 1968 *Magnetism and Magnetic Materials Digest*. The *Digest* is published annually and contains a survey of the technical literature of the preceding year. *Magnetism and Magnetic Materials—1968 Digest* will contain 21 chapters of general subjects such as Neutron Diffraction, Spin Configuration and Magnetic Transitions, Properties of Non-Metals, Thin Films, and Magnetic Domains. Each chapter will consist of a bibliography, materials index, and a brief, noncritical evaluation of all papers published during the previous year within the scope of each author's chapter. Dr. Bennett's chapter will deal with all papers published in 1967 relating to nuclear magnetism in exchange-coupled electron-magnetic materials. Some of the topics included are: Hyperfine interactions, nuclear specific heat, Mössbauer effect, nuclear magnetic resonance, Knight shift, s-d interaction, and temperature dependence of spontaneous magnetization. Approximately 185 papers will be reviewed in this chapter alone.

The 1968 *Digest* will be published by the Academic Press, and will be sold at the 14th Annual Conference of Magnetism and Magnetic Materials in November 1968.

Photoabsorption Cross Section Data

JILA Information Center Report No. 5, "Bibliography of Photoabsorption Cross Section Data," by L. J. Kieffer, provides references to published low energy atomic collision data dealing with cross sections of absorption and ionization coefficients for wavelength regions of continuous absorption. The bibliography is divided into three main sections. The first section describes the data under references according to a hierarchy of descriptors. The second section lists title, authors, and complete refer-

ences for the papers cited. The third section is an alphabetical author index. Copies of the bibliography are available from the JILA Information Center, University of Colorado, Boulder, Colo. 80302.

AMPIC Issues New Bibliography

ORNL-AMPIC-10, *Bibliography of Atomic and Molecular Processes for July-December 1967*,³ published in June 1968, is the eighth in a series of bibliographies published by the Atomic and Molecular Processes Information Center (AMPIC) at Oak Ridge National Laboratory. The Center is jointly sponsored by the U.S. Atomic Energy Commission and the NBS Office of Standard Reference Data. This annotated bibliography contains references of interest to atomic and molecular processes research. Bibliographic sources consist of eighty scientific journals and five abstract journals. As in the previous bibliographies of this series, references are classified into fourteen major categories with appropriate subcategories, and are entered alphabetically in each category with the reactants or the atomic and molecular system of interest.

Chemical Kinetics

Compilation, evaluation, and tabulation of numerical data in the field of chemical kinetics presents a number of special problems. By definition, the system is changing in composition—the reaction mechanism may be uncertain, or may change with temperature or other parameters; catalysts, wall-effects and other local influences may be significant. Previous attempts to present kinetic data in tabular form have found the difficulties substantial. One such attempt was NBS Circular 510, *Tables of Chemical Kinetics—Homogeneous Reactions*, issued with two supplements, and prepared under the direction of N. Thon and Charles Stauffer.

To obtain advice on a program which might avoid some of these problems, the NBS Office of Standard Reference Data sought the counsel of the NAS-NRC Committee on the Kinetics of Chemical Reactions. The recommendations of the Committee recognized the difficulties inherent in any attempt to evaluate and compile the large amount of numerical data published on chemical reaction rates. The Committee suggested a program of critical review monographs on narrow topics, to be written by qualified specialists. Their purpose would be to provide comprehensive coverage, with emphasis on the quantitative aspects and with extensive bibliographies.

A number of critical reviews have been started and some are completed. Experience to date indicates that the critical review approach is valuable. Additionally, rate constant data were carefully selected for compilation and critical evaluation in areas of bimolecular chemical reactions. These kinetic data have now been published in tabular form. The assembly and publication of data sheets

describing the kinetics of individual chemical reactions are also being encouraged. In all these efforts it has become apparent that the author must be careful to limit the scope of his topic to avoid being overwhelmed by the quantity of literature he must read and analyze.

It has also become clear that both the review authors and the user public can be helped greatly by the establishment of information and data centers which function to:

- Help stimulate qualified prospective authors to critically evaluate kinetic data in which they have expertise;
- provide authors of monographs with bibliographic services and assistance;
- maintain coverage of the scientific literature on a current basis;
- store and classify the data and bibliographic content of critical review monographs;
- provide information to the scientific public on the basis of items (c) and (d).

Two data centers have been established by the Office of Standard Reference Data: the NBS Chemical Kinetics Information Center, acting in a general capacity (*NSRDS News*, September 1966),⁴ and the University of Notre Dame Radiation Chemistry Data Center (*NSRDS News*, January 1968).⁵ At present, these centers are performing services listed as (b) and (c) above, and are providing some limited information services to the public as well. Establishment of additional centers and arrangements for additional critical review monographs have been hampered by lack of funds. The support of the Department of Defense's Advanced Research Projects Agency has provided means for partial support of the Chemical Kinetics Information Center. The Atomic Energy Commission has shared in supporting the Radiation Chemistry Data Center.

Reaction Rate Newsletter

Workers in chemical kinetics may be interested in receiving the *Defense Atomic Support Agency Information and Analysis Center Newsletter*, which provides summaries of current progress reports in the reaction rate field. The newsletter contains privileged information which should be considered preliminary in nature and subject to possible change; it should not be cited in any publication without prior approval. Persons wishing to subscribe should send their requests to DASA Information and Analysis Center, General Electric—TEMPO, 816 State St., Santa Barbara, Calif. 93102.

¹ Available from the Superintendent of Documents, U.S. Government Printing Office, Washington, D.C. 20402, for the price indicated.

² Hilsenrath, J., Ziegler, G. G., Messina, C. G., Walsh, P. J., and Herbols, R. J., *OMNITAB—A Computer Program for Statistical and Numerical Analysis*, NBS Handbook 101, U.S. Government Printing Office, Washington, D.C. 20402, Mar. 4, 1966 (\$3).

³ Available from the Atomic and Molecular Processes Information Center, Oak Ridge National Laboratory, P.O. Box Y, Oak Ridge, Tenn. 37831.

⁴ *NSRDS News*, NBS Tech. News Bull. 50, No. 9, 166–168 (September 1966).

⁵ *NSRDS News*, NBS Tech. News Bull. 52, No. 1, 14–16 (January 1968).